

Cluster coherent potential approximation for electronic structure of disordered alloys

M. S. Laad^{*1} and L. Craco²

¹*Department of Physics, Loughborough University, LE11 3TU, UK*

²*Institut für Theoretische Physik, Universität zu Köln, 77 Zùlpicher Strasse, D-50937 Köln, Germany*

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We extend the single-site coherent potential approximation (CPA) to include the effects of non-local disorder correlations (alloy short-range order) on the electronic structure of random alloy systems. This is achieved by mapping the original Anderson disorder problem to that of a selfconsistently embedded cluster. This cluster problem is then solved using the equations of motion technique. The CPA is recovered for cluster size $N_c = 1$, and the disorder averaged density-of-states (DOS) is always positive definite. Various new features, compared to those observed in CPA, and related to repeated scattering on pairs of sites, reflecting the effect of SRO are clearly visible in the DOS. It is explicitly shown that the cluster-CPA method always yields positive-definite DOS. Anderson localization effects have been investigated within this approach. In general, we find that Anderson localization sets in before band splitting occurs, and that increasing partial order drives a continuous transition from an Anderson insulator to an incoherent metal.

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I. INTRODUCTION

The problem of atomic short-range order (SRO) and its effect on the character of electronic dynamics has been studied for many years now. It is relevant to the detailed understanding of the conditions under which a transition from metallic to an Anderson localized (AL), disordered insulator occurs with increasing disorder strength [1]. In the $d = \infty$ limit, the well-known coherent potential approximation (CPA) [2] provides the *exact* solution of this Anderson disorder problem. However, by construction, CPA cannot access specific effects (quantum interference from short-ranged scattering potentials) leading to AL behavior. Such an endeavor demands explicit incorporation of the *dynamical* effect of SRO on carrier propagation in a disordered system, and thus, a cluster generalization of CPA. Such attempts have indeed been carried out [3,4], but are extremely cumbersome numerically. Additionally, they do not always guarantee the correct analyticity properties of the Green's functions: the few which do succeed in this respect, like the travelling cluster approximation (TCA) [4] and the dynamical cluster approximation (DCA) [5] are extremely tedious technically. Further, the study of the effects of short-range order (SRO) on carrier dynamics has, to our best knowledge, never been attempted using these approaches. It is obvious that attempting to tackle the harder problem of atomic (or doping induced) SRO along with arbitrarily strong local electronic correlations, not to mention important aspects like multi-orbital character of realistic transition metal-based oxide systems, with these approaches would be extremely numerically time-consuming. Given this, it is imperative to develop semi-analytical routes as far as possible, resulting in much better (and easier) numerical tractability.

On the other hand, many important results have been gleaned from field-theoretic studies of the Anderson tran-

sition. Perturbative renormalization group (RG) [6] approaches and extensions thereof, work in the weak disorder regime, and are a priori inapplicable in the non-perturbative regime where the Anderson-Mott MIT would be expected to occur in the $3d$ case. As a result, well-defined precursors of the MIT are observed even at very high temperatures, as experimentally demonstrated [7] in many systems in the form of scaling behavior of various quantities, breakdown of Matthiessen rule and the Mooij correlation. Thus, while the perturbative ($d + \epsilon$) [6] approaches have indeed provided wealth of information, such approaches are insufficient at strong coupling, which is precisely the regime of interest for doped TMO systems, as well as systems like strongly interacting two-dimensional electron systems (in *Si* MOSFETs [8]) which have been found to undergo insulator-metal transitions. This is because one is always *effectively* in the strong disorder regime in strongly correlated electronic systems, where the renormalized one-electron band width is very small (caused by Hubbard band-narrowing) in the correlated metal (or Mott insulating states, where the band splitting *a la* Mott-Hubbard mechanism occurs). Consideration of such cases is out of bounds with perturbative approaches, and this requires development of genuinely non-perturbative approaches which should be capable of:

(i) extending the CPA to access Anderson localization effects, and,

(ii) having sufficient flexibility to incorporate effects of Mott-Hubbard physics via dynamical mean-field (DMF) or cluster-DMF approaches.

In this paper, we devise a new *cluster*-CPA technique that satisfies the above requirements. It is extremely simple to implement (requires only the solution of N_c coupled, non-linear equations for the Green's function for a cluster with N_c sites), captures the *intracluster* correlations exactly, and is suited to further

improvements (larger cluster size, incorporation of Mott-Hubbard physics). As we will show, it also reproduces the exact CPA limit [2] for the single-site cluster ($d = \infty$).

The CPA is tailor-made to describe electron dynamics in a system with purely diagonal disorder when correlations between spatially separated disorder scatterers can be ignored, a situation which is formally exact in $d = \infty$. Extensions to include off-diagonal (hopping) disorder within the CPA framework have been proposed [3] by a variety of authors. Here, we will propose a different (related to non-local CPA) Green's function technique. Using the EOM technique, we explicitly include *dynamical* effects of arbitrarily strong scattering from short-range correlated disorder potentials. In the process, we will make explicit contact with the problem of Anderson localization in disordered systems.

II. MODEL AND SOLUTION

The first step is the construction of a suitable cluster model Hamiltonian incorporating *diagonal* disorder. Motivated by results of Ref. [9], we generalize the Anderson disorder problem to finite dimensions by mapping the full Anderson disorder model,

$$H = -t \sum_{\langle i,j \rangle} (c_i^\dagger c_j + h.c.) + \sum_i v_i n_i, \quad (1)$$

to an effective model of a cluster of N_c sites embedded in an effective (dynamical) bath with a *complex* self-energy (matrix of size N_c^2). Here, we assume a binary alloy distribution for disorder, $P(v_i) = (1-x)\delta(v_i - v_A) + x\delta(v_i - v_B)$, and further, that $\langle v_i v_j \rangle - \langle v_i \rangle \langle v_j \rangle = f_{ij} \equiv C$, a constant parameter. Strictly speaking, the SRO encoded in f_{ij} is a function of x , temperature and other variables depending on the specific physical situation under consideration, and in real materials, this dependence should be explicitly taken into account.

In contrast to CPA, the method described below is tailor made to capture the dynamical effects of repeated scattering from a cluster of sites, which are correlated in a manner described by f_{ij} over the cluster length scale. To proceed, we start with the embedded cluster Hamiltonian,

$$H = -t \sum_{\alpha} (c_0^\dagger c_{\alpha} + h.c.) + v \sum_{\alpha} x_{\alpha} n_{\alpha} + t \sum_{k,\alpha} e^{ik \cdot R_{\alpha}} (c_{\alpha}^\dagger c_k + h.c.), \quad (2)$$

where $0, \alpha = 1, \dots, z$ denote a central site 0 coupled (via t) to z nearest neighbors on a $d = z/2$ dimensional lattice, and the last term describes the hybridization of the boundary of the chosen cluster with an effective medium

(conduction electron bath function) that has to be self-consistently determined by a suitable imbedding procedure. We describe the details in course of the derivation below.

Defining the diagonal and off-diagonal propagators on the cluster as $G_{00}(\omega) = \langle c_0; c_0^\dagger \rangle$, $G_{\alpha 0}(\omega) = \langle c_{\alpha}; c_0^\dagger \rangle$, $G_{\alpha\alpha}(\omega) = \langle c_{\alpha}; c_{\alpha}^\dagger \rangle$, we start with the equation of motion (EOM) for $G_{00}(\omega)$:

$$\omega G_{00}(\omega) = 1 + t \sum_{\alpha} G_{\alpha 0}(\omega) + v \langle x_0 c_0; c_0^\dagger \rangle. \quad (3)$$

Notice the appearance of a higher-order GF on the rhs of Eq. (3). It is naturally interpreted as the probability amplitude for having an electron at a site 0 with disorder potential v . Its EOM reads,

$$(\omega - v) \langle x_0 c_0; c_0^\dagger \rangle = \langle x_0 \rangle + t \sum_{\alpha} \langle x_0 c_{\alpha}; c_0^\dagger \rangle. \quad (4)$$

The EOM for $G_{\alpha 0}(\omega)$ on the rhs of Eq. (3) reads,

$$\omega G_{\alpha 0}(\omega) = v \langle x_{\alpha} c_{\alpha}; c_0^\dagger \rangle + t G_{00}(\omega) + t \sum_{j \neq \alpha} G_{j 0}(\omega), \quad (5)$$

and in a way similar to that leading to Eq. (4), we obtain,

$$(\omega - v) \langle x_{\alpha} c_{\alpha}; c_0^\dagger \rangle = t \langle x_{\alpha} c_0; c_0^\dagger \rangle + t \sum_{j \neq \alpha} \langle x_{\alpha} c_j; c_0^\dagger \rangle. \quad (6)$$

Continuing along with identical lines for the various higher-order GFs generated in Eqs. (3-5) give us

$$\begin{aligned} \omega \langle x_0 c_{\alpha}; c_0^\dagger \rangle &= v \langle x_0 x_{\alpha} c_{\alpha}; c_0^\dagger \rangle + t \langle x_0 c_0; c_0^\dagger \rangle \\ &+ t \sum_{j \neq \alpha} \langle x_0 c_j; c_0^\dagger \rangle, \end{aligned} \quad (7)$$

$$\omega \langle x_{\alpha} c_0; c_0^\dagger \rangle = \langle x_{\alpha} \rangle + v \langle x_{\alpha} x_0 c_0; c_0^\dagger \rangle + t \langle x_{\alpha} c_{\alpha}; c_0^\dagger \rangle, \quad (8)$$

$$\begin{aligned} (\omega - v) \langle x_0 x_{\alpha} c_{\alpha}; c_0^\dagger \rangle &= t \langle x_0 x_{\alpha} c_0; c_0^\dagger \rangle \\ &+ t \sum_{j \neq \alpha} \langle x_0 x_{\alpha} c_j; c_0^\dagger \rangle \end{aligned} \quad (9)$$

and,

$$(\omega - v) \langle x_{\alpha} x_0 c_0; c_0^\dagger \rangle = \langle x_0 x_{\alpha} \rangle + t \langle x_0 x_{\alpha} c_{\alpha}; c_0^\dagger \rangle. \quad (10)$$

Finally,

$$(\omega - \epsilon_k) \langle A_{0\alpha} c_k; c_0^\dagger \rangle = t_k \langle A_{0\alpha} c_{\alpha}; c_0^\dagger \rangle; \quad (11)$$

where $A_{0\alpha} = 1, x_0, x_\alpha, x_0x_\alpha$ for the various types of Green functions which couple the bath back to the cluster (see above), and $\langle x_{0\alpha} \rangle \equiv \langle x_0x_\alpha \rangle$ is the non-local correlation function of the disorder potential over the cluster length scale (scaling like $1/d$ in d dimensions). For a single site cluster, we recover the *exact* CPA result using the EOM for $G_{00}, G_{k0}, \langle x_0c_0; c_0^\dagger \rangle$ and $\langle x_0c_k; c_0^\dagger \rangle$ only. Indeed, the local Green's function at the site 0 is easily seen to be,

$$G_{00}(\omega) = \frac{1 - \langle x_0 \rangle}{\omega - \Delta(\omega)} + \frac{\langle x_0 \rangle}{\omega - v - \Delta(\omega)}, \quad (12)$$

with $\Delta(\omega) = \sum_k \frac{|t_k|^2}{\omega - \Sigma(\omega) - \epsilon_k}$, which is exactly the CPA result.

In our cluster generalization, after a long and somewhat tedious algebra, we finally find,

$$G_{00}(\omega) = \frac{1 + v \langle x_0c_0; c_0^\dagger \rangle + (v/t)F_2(\omega) \langle x_\alpha c_\alpha; c_0^\dagger \rangle}{\omega - zF_2(\omega)} \quad (13)$$

and,

$$G_{\alpha 0}(\omega) = \frac{1}{\omega - \Delta(\omega)} \frac{v \langle x_\alpha c_\alpha; c_0^\dagger \rangle + t(1 + v \langle x_0c_0; c_0^\dagger \rangle)}{\omega - zF_2(\omega)} \quad (14)$$

where,

$$v \langle x_0c_0; c_0^\dagger \rangle = \frac{v \langle x_0 \rangle + (v/t)^2 \langle x_0x_\alpha \rangle \frac{F_1(\omega)F_2(\omega)}{\omega - v - F_1(\omega)}}{\omega - v - F_2(\omega)} \quad (15)$$

and,

$$\langle x_\alpha c_\alpha; c_0^\dagger \rangle = t^{-1} F_1(\omega) \langle x_\alpha c_0; c_0^\dagger \rangle, \quad (16)$$

with

$$\langle x_\alpha c_0; c_0^\dagger \rangle = \frac{\langle x_\alpha \rangle - \langle x_0x_\alpha \rangle}{\omega - F_1(\omega)} + \frac{\langle x_0x_\alpha \rangle}{\omega - v - F_1(\omega)}. \quad (17)$$

Here, $F_1(\omega) \equiv \frac{t^2}{\omega - v - \Delta(\omega)}$ and $F_2(\omega) \equiv \frac{t^2}{\omega - \Delta(\omega)}$. Finally, the bath function, $\Delta(\omega)$ is computed from the equation [11,12],

$$G_{00}(\omega) = \int_{-W}^{+W} \frac{\rho_0(\epsilon) d\epsilon}{G_{00}^{-1}(\omega) + \Delta(\omega) - \epsilon}. \quad (18)$$

with $\Delta(\omega) = t^2 G_{00}(\omega)$ for the Bethe lattice. At this point, one can show that the cluster-CPA technique developed above always yields positive-definite local DOS, defined by $\rho(\omega) = -\text{Im}G_{00}(\omega)/\pi$. To show this explicitly, we observe that $G_{00}(\omega)$ can be brought to a convenient mathematical form by simple algebraic manipulations

$$G_{00}(\omega) = \frac{1 - \langle x_0 \rangle}{\omega - F_2(\omega)} + \frac{\langle x_0 \rangle}{\omega - v - F_2(\omega)} - \left[\frac{\langle x_\alpha \rangle - \langle x_0x_\alpha \rangle}{\omega - F_2(\omega)} + \frac{\langle x_0x_\alpha \rangle}{\omega - v - F_2(\omega)} \right] + \frac{\langle x_\alpha \rangle - \langle x_0x_\alpha \rangle}{\omega - F_1(\omega)} + \frac{\langle x_0x_\alpha \rangle}{\omega - v - F_1(\omega)} \quad (19)$$

The first step in the derivation is to notice that each of the numerators is always positive definite by definition. Clearly, to show that $\rho(\omega)$ is always positive definite, we have now only to show that $\text{Im}\Delta(\omega) \leq 0$. From the EOM technique used above, $\Delta(\omega) = \sum_k \frac{t_k^2}{\omega - \epsilon_k}$. A straightforward calculation shows that $\text{Im}\Delta(\omega) \leq 0$ for any choice of the unperturbed DOS, $\rho_0(\epsilon) \geq 0$. Substitution in $G_{00}(\omega)$ above immediately shows that the disorder averaged DOS is always positive definite (clearly, self-consistency does not modify this conclusion).

Few clarifications concerning the physical meaning of the set of equations is in order at this point. First, we notice that the carrier dynamics is an explicit function of the higher-order (in $1/d$) SRO correlator, $\langle x_0x_\alpha \rangle$. It is also easy to check that the system of equations are exact both in the band and the atomic limit, and the CPA result is readily recovered for the single-site cluster. To interpret the meaning of the bath function, $\Delta(\omega)$ in our approach, we begin by observing that one can view *any* selfconsistent cluster approximation as being a valid description in a regime with short-ranged order on the cluster length scale (analogous to the single site approximation being formally exact at mean field level). An exact solution of the problem implies consideration of an infinite cluster, and, of course, is an insoluble problem. Our choice for $\Delta(\omega)$ above is then linked to the mathematical consideration of short-ranged correlations over the cluster length scale only, or, equivalently, to the consideration of dynamical effects of repeated scattering by a cluster consisting of a central site plus its z nearest neighbors only. The effects of non-local SRO appears explicitly in the bath function $\Delta(\omega)$ (i.e, in Eqn. (18)) via $G_{00}(\omega)$ as defined in Eqn. (13) with its explicit dependence on f_{ij} . It follows that the approach describes carrier dynamics in a situation where the carrier mean free path is of the order of the size of the chosen cluster ($l \simeq a$, the lattice constant for our cluster) in a fully selfconsistent way (see below), one step beyond the CPA where $l = 0$.

It is interesting to notice that $G_{00}(\omega), G_{\alpha 0}(\omega)$ can be (formally) analytically expressed in terms of the corresponding diagonal and off-diagonal cluster self-energies $\Sigma_{00}(\omega), \Sigma_{\alpha 0}(\omega)$ for $d = 1, 2, \dots, \infty$, as well as on certain special lattices. The above set of equations then constitute a closed set of simultaneous non-linear equations for the two self-energies, and are solved self-consistently to yield the renormalized (by disorder) DOS at the central site, $\rho(\omega) = -\frac{1}{\pi} \text{Im}G_{00}(\omega)$.

The alloy correlation function (describing SRO) is given by $\langle x_0 x_\alpha \rangle = \langle x_0 \rangle \langle x_\alpha \rangle + C_{0\alpha}$ in the general case, with $C_{0\alpha}$ encoding complete information about order-disorder instabilities in the alloy. It is important to notice that the *dynamical* effect of strong scattering by these short-ranged correlations ($C_{0\alpha}$) on the electronic self-energy is explicitly included within our formulation above. In particular, the electron can undergo repeated scattering on the atomic sites within the chosen cluster, and, depending upon the degree and character of SRO (see below), can be localized due to interference effects coming from repeated scattering from spatially separated centers; i.e. via Anderson localization. To address the issue of Anderson localization in our NLCPA scheme, we follow Economou *et al.* [10] and use the localization function defined by:

$$L(\omega) = Kt \left| G_{00}(\omega) - \frac{G_{0\alpha}(\omega)G_{\alpha 0}(\omega)}{G_{00}(\omega)} \right|, \quad (20)$$

where electronic eigenstates with energy ω satisfying:

- $L(\omega) > 1$ define *extended* states,
- $L(\omega) < 1$ define Anderson localized states, and,
- $L(\omega) = 1$ defines the mobility edge.

Here, K is the connectivity of the lattice. The formalism developed above thus allows a complete determination of the Anderson transition and its dependence on lattice structure, type of SRO, and band-filling.

III. NUMERICAL RESULTS AND DISCUSSION

In this section, we describe the results obtained from the numerical solution of the self-consistent set of coupled nonlinear equations derived in the previous section. Since we are interested in generic effects of atomic SRO on carrier dynamics, we choose the semicircular unperturbed DOS $\rho_0(E) = \frac{2}{\pi W^2} \sqrt{W^2 - E^2}$ as an approximation to the actual DOS for a three dimensional cubic lattice [11]. This leads to a considerable simplification in the numerics without affecting the generic features qualitatively. We work with $W = 1.424$ eV and study the fully renormalized DOS, $\rho(\omega)$ and $L(\omega)$ as functions of the alloy composition $y = (\langle x_0 \rangle / (1 - \langle x_0 \rangle))$, the atomic SRO parameter $C_{0\alpha}$ and the disorder strength v for a half-filled band.

We begin with the symmetric case with $y = 1$, and extreme random disorder, i.e. $C_{0\alpha} = 0$ or $\langle x_{0\alpha} \rangle = \langle x_0 \rangle \langle x_\alpha \rangle$. In $d = \infty$, this corresponds to the CPA, with the metal-insulator transition occurring *continuously* at $v \geq W$. Inclusion of SRO drastically changes the picture. The M-I transition now occurs much earlier. In

fact, the band split regime occurs for $v/W \geq 1/4$. However, states near and at the band center become Anderson localized *before* the band splits (Fig. 1) and the metal (incoherent)- Anderson insulator transition is continuous. For $v < v_c$, the incoherent metal has a very similar character (breakdown of the quasiparticle) to that found in $d = \infty$ (CPA). It is also clear that the configuration averaged single particle DOS shows no anomalies across the Anderson localization transition, in agreement with well known [13] arguments.

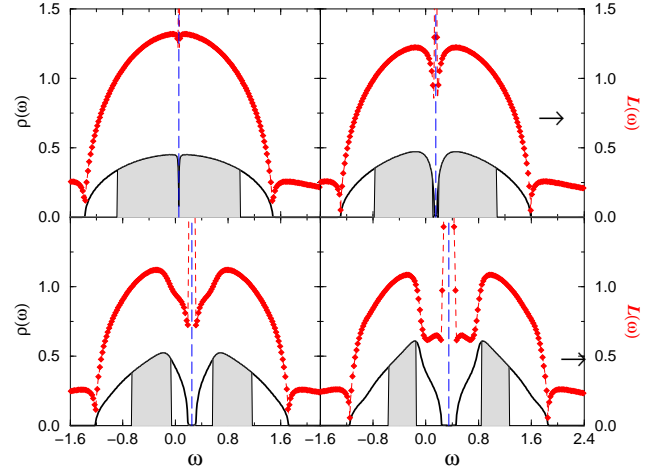


FIG. 1. Cluster-CPA DOS the binary-alloy distribution in the extreme SRO limit on a Bethe lattice for $\langle x_0 \rangle = 0.5$, $\langle x_{0\alpha} \rangle = 0.0$ and various values of the local disorder potential, $v = 0.1, 0.2, 0.3, 0.4$. Shaded regions define extended states, and unshaded regions define Anderson localized states.

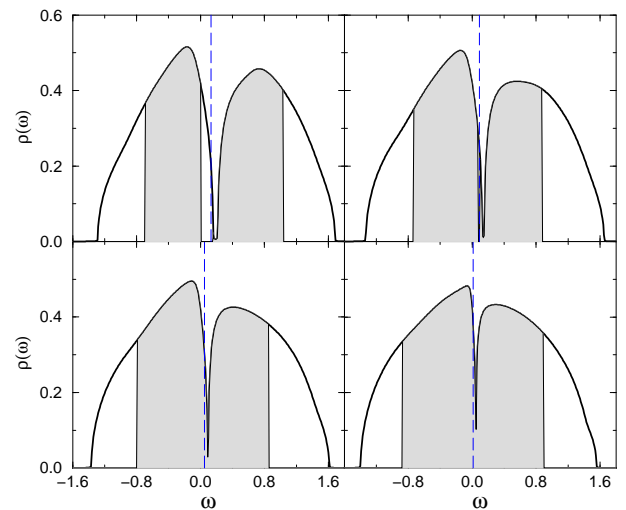


FIG. 2. (Cluster-CPA DOS on a Bethe lattice for $\langle x_{0\alpha} \rangle = 0.0$, $v = 0.5$ and different alloy concentrations, $\langle x_0 \rangle = 0.4, 0.3, 0.2, 0.1$.

In Fig. 2, we show the effect of changing the alloy composition on the critical value of v needed to split the band. For the case $y = 2/3$ (i.e., $\langle x_0 \rangle = 0.4$), a larger $v_c = 0.5$ is required to localize states at E_F , and it increases to $v_c = 0.85$ for $y = 3/7$ ($x = 0.3$). This Anderson insulating state (notice that the Fermi level, denoted by the vertical lines in our plots, lies in the region of localized states) is explicitly related to our inclusion of the effect of carrier scattering on short-ranged intersite atomic correlations $C_{0\alpha} = C$) and is never observed in the CPA solution ($d = \infty$), which always predicts an incoherent metal for a (half-filled band) particle-hole asymmetric disorder distribution. A continuous transition from an Anderson localized insulator to an incoherent metal is clearly seen upon decreasing y for a fixed disorder strength.

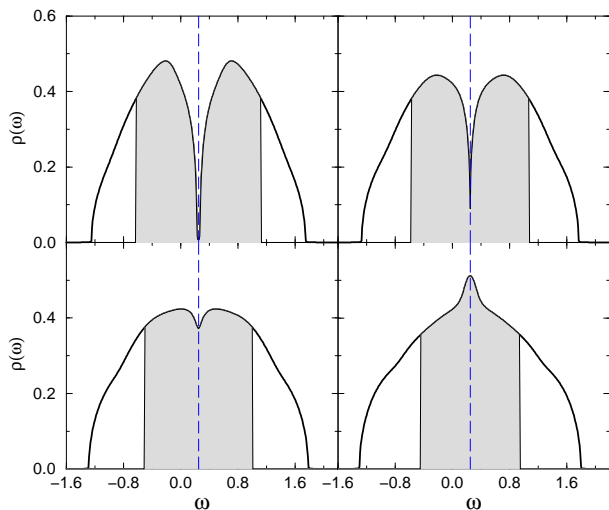


FIG. 3. Effect of partial SRO on the Cluster-CPA DOS for a Bethe lattice with $\langle x_0 \rangle = 0.5$, $v = 0.5$ and $\langle x_{0\alpha} \rangle = 0.1, 0.2, 0.3, 0.4$.

Next, we focus on the effect of varying the SRO parameter on the electronic structure. In Fig. 3, we show the DOS for $v = 0.5$ for different values of $\langle x_{0\alpha} \rangle = 0.1, 0.2, 0.3, 0.4$. Clearly, introducing partial order (actually, this corresponds to *increasing* $C_{0\alpha}$) results in increased tendency to itinerance, moving E_F out of the region of localized states. The AL insulator to incoherent metal transition is clearly observed with increasing $C_{0\alpha}$, and is a concrete illustration of an insulator-metal transition driven by the degree of atomic SRO (partial order) in a system. Clearly, increasing partial order (notice that increasing $C_{0\alpha}$ corresponds to increasing the probability of having the *same* potential on the cluster sites) reduces the localizing effect of strong (repeated) intracluster disorder scattering, driving the I-M transition via increased itinerance. The situation is very analogous to the case where the pure Anderson disorder model is supplemented by additional short-range correlations in

the hopping [14], where increasing the off-diagonal randomness drives an insulator-metal transition for a fixed diagonal disorder strength.

Qualitatively similar behavior is seen for an asymmetric alloy distribution. In Fig. 4, we show the DOS for $v = 0.5$ and $y = 3/7$ (i.e., $\langle x_0 \rangle = 0.3$). Interestingly, the spectrum shows additional features, but the AL insulator-metal transition with increasing $C_{0\alpha}$ follows the trend for the symmetric ($y = 1$) case.

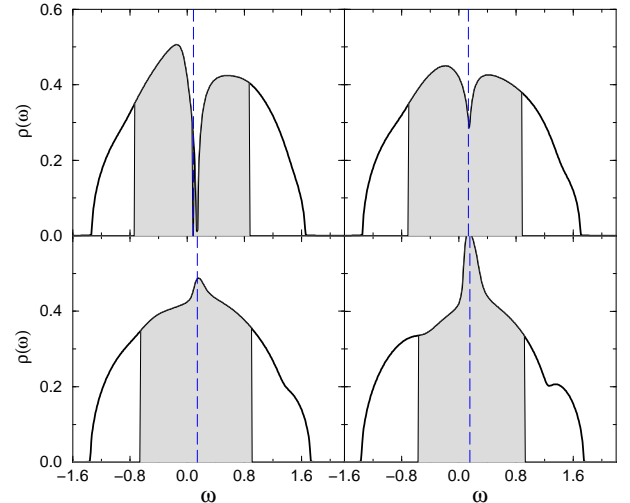


FIG. 4. Effect of partial SRO on the Cluster-CPA DOS for a Bethe lattice with $\langle x_0 \rangle = 0.3$, $v = 0.5$ and $\langle x_{0\alpha} \rangle = 0.0, 0.1, 0.2, 0.3$.

Increasing the ratio v/W reveals rich structures in the DOS. In Fig. 5, we show the one-electron DOS for $v = 1.5$ with $\langle x_{0\alpha} \rangle = 0.0, 0.1, 0.2, 0.3$. Next, we turn our attention to Fig. 6, which shows the evolution of the DOS for the asymmetric alloy distribution with $\langle x_0 \rangle = 0.3$ for the same parameters. In this case, we are already in the split-band regime. Very rich structure is seen in the results. For comparison, we know that the corresponding DOS obtained for these cases within CPA ($d = \infty$, not shown) shows a split band structure with only upper- and lower “Hubbard” bands. Obviously, CPA is incapable of resolving the fine structure in the DOS originating from repeated scattering between spatially separated scattering centers. The rich structures seen in the cluster generalization correspond partially to these effects, and can be traced back to the spectrum of eigenstates of the isolated cluster. In fact, the multiple sub-bands can easily be shown to be centered around eigen-energies of the isolated cluster for the case of the symmetric alloy distribution with $f_{0\alpha} = 0$. However (Figs. 5-6), in the general case with $f_{0\alpha} \neq 0$, one sees eight or nine distinct sub-band structures. We interpret the additional structures as arising from atomic SRO (non-zero $f_{0\alpha}$); in particular from “shake-up” effects originating from strong resonant

scattering of carriers (from the atomic SRO) from cluster sites. For comparison, we remark that coupling the two-site cluster to the “bath” (rest of the lattice) via second order processes in the hopping (corresponding to the “Hubbard I” approximation for the cluster) is incapable of accessing SRO effects in a consistent way. In particular, in addition to violating the Hubbard sum rules [15], it cannot yield “shake-up” features in the DOS, always yielding *only* six bands centered around the eigenvalues of the 2-site cluster, and broadened by an amount $O(t)$. This discussion shows the importance of treating the effects of *both* itinerance (via $\Delta(\omega)$) and the (incoherent) resonant scattering on the same footing, and reveals the weaknesses inherent in uncontrolled approximations.

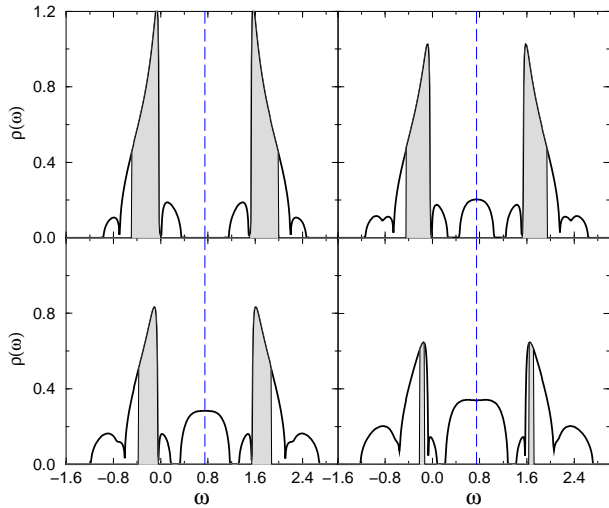


FIG. 5. Cluster-CPA DOS for $\langle x_0 \rangle = 0.5$, $v = 1.5$ and $\langle x_{0\alpha} \rangle = 0.0, 0.1, 0.2, 0.3$.

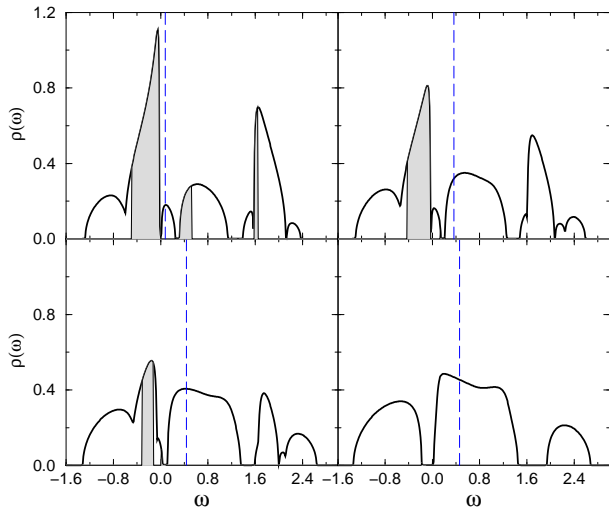


FIG. 6. Cluster-CPA DOS for $\langle x_0 \rangle = 0.3$, $v = 1.5$ and $\langle x_{0\alpha} \rangle = 0.0, 0.1, 0.2, 0.3$.

Additional interesting features observed from the calculations deserve comments. We clearly observe that the localization function $L(\omega)$ shows non-analytic behavior near each subband edge, but no non-analyticities across the mobility edge. More detailed characterization of the Anderson insulator-metal transition requires a detailed study of the two-particle responses [16] (density correlations, optical conductivity) and is left for future work.

Our results show some resemblance to those obtained by Rowlands *et al.* [17] for the same model (in 1d) using the Korringa-Kohn-Rostoker Non-Local Coherent Potential Approximation (NLCPA) employing the dynamical cluster approximation (DCA). However, no attempt has been made there to study Anderson localization. Further, our treatment of partial SRO is very different from theirs. It is worth pointing out that our results, along with the NLCPA ones, are quite different from those obtained by Jarrell *et al.* [5]. However, we are presently unable to quantify the reasons behind these differences.

We emphasize that the approach developed here has a wide applicability to various problems where the effect of atomic (chemical), magnetic, Jahn-Teller, etc., SRO on the character of carrier dynamics is an important issue. In particular, it should be applicable to the problem of electronic structure of disordered TM alloys [18], and to more recent cases such as hole-doped manganites [19], where a plethora of experimental work clearly demonstrates the importance of such effects in a correlated environment. Applications to such systems is in progress and will be reported elsewhere.

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* Electronic Address: M.S.Laad@lboro.ac.uk

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